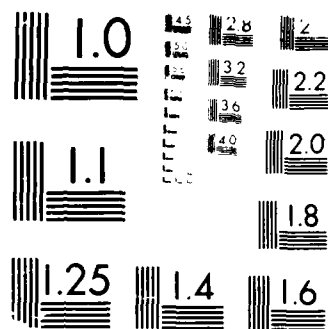


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**Optimisation of the Thermoelectric Figure of Merit of  
Modified Silicon Germanium Alloys**

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## OPTIMISATION OF THE FIGURE OF MERIT OF MODIFIED SILICON GERMANIUM ALLOYS

### 1. Introduction

Alloys of silicon and germanium are established semiconductor materials for use in high temperature thermoelectric conversion systems. The conversion efficiency of a thermoelectric device depends, among other things, upon the material properties of the thermoelements through the so-called figure of merit  $Z = \alpha^2 \sigma / \lambda$  where  $\alpha$  is the Seebeck coefficient,  $\sigma$  the electrical conductivity and  $\lambda$  the total thermal conductivity. It has been predicted and demonstrated experimentally that the lattice thermal conductivity  $\lambda_L$  of semiconductor alloys can be substantially reduced through the use of very small grain size compacted material (1). Consequently, if the electrical parameters remain unchanged, this reduction in  $\lambda_L$  would result in a higher figure of merit and an improved conversion efficiency. However, apart from one report, in which GaP (2) was added to silicon-germanium alloy, available data indicate that the observed reduction in  $\lambda$  is accompanied by a degradation in electrical behaviour.

Evidently, it is of considerable interest to any project associated with the development of improved thermoelectric materials based on silicon germanium alloys to explore the behaviour of  $\alpha$  and  $\sigma$  with alloy composition and with carrier concentration, and to identify the conditions which optimise the power factor  $\alpha^2 \sigma$ .

Such an investigation would provide a foundation for a subsequent programme of work into the role of additives such as GaP in apparently enhancing the thermoelectric figure of merit of the materials.

The development of a comprehensive and realistic theoretical model which provides a description of the electrical properties of the silicon germanium alloy system is difficult and is best approached in stages, commencing with a working model and progressing to more realistic models of increased complexity. The proposed programme of work is based on these considerations.

## 2 Proposed Programme of Work

- (i) Study the variation of  $\alpha^2\sigma$  with reduced Fermi energy and carrier concentration for a range of specific alloy compositions.
- (ii) Undertake a literature survey with the view to exploring changes in the band structure of silicon germanium alloys with change in composition from pure germanium to pure silicon; identify the effect of these changes on  $\alpha$  and  $\sigma$ .
- (iii) As stage (i), but including the effect of non-parabolic energy bands in the theoretical model.
- (iv) Develop an idealized model and explore the variation of  $\alpha^2\sigma$  with number of valleys.
- (v) Identify the parameters and conditions which optimise the material power factor  $\alpha^2\sigma$ .

## 3. References

1. D. M. Rowe, V. S. Shukla and N. Savvides, Nature 290, 765 (1981).
2. R. K. Pisharody and L. P. Garvey in Proceedings of 13th IECEC (IEEE Publishing Service, New York 1978), p.1963.

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